

Non-equilibrium steady state and subgeometric ergodicity for a chain of three coupled rotors

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Abstract

We consider a chain of three rotors (rotators) whose ends are coupled to stochastic heat baths. The temperatures of the two baths can be different, and we allow some constant torque to be applied at each end of the chain. Under some non-degeneracy condition on the interaction potentials, we show that the process admits a unique invariant probability measure, and that it is ergodic with a stretched exponential rate. The interesting issue is to estimate the rate at which the energy of the middle rotor decreases. As it is not directly connected to the heat baths, its energy can only be dissipated through the two outer rotors. But when the middle rotor spins very rapidly, it fails to interact effectively with its neighbours due to the rapid oscillations of the forces. By averaging techniques, we obtain an effective dynamics for the middle rotor, which then enables us to find a Lyapunov function. This and an irreducibility argument give the desired result. We finally illustrate numerically some properties of the non-equilibrium steady state.

1 Introduction

Hamiltonian chains of mechanical oscillators have been studied for a long time. Several models describe a linear chain of masses, with polynomial *interaction* potentials between adjacent masses, and *pinning* potentials which tie the masses down in the laboratory frame. Under the assumption that the interaction is stronger than the pinning, it was shown in [6] that the model has an invariant probability measure when the chain is attached at each extremity to two heat baths at different temperatures. That paper, and later developments, see *e.g.*, [4], relied on analytic arguments, showing in particular that the infinitesimal generator has compact resolvent in a suitable function space.

Two elements were added later in the paper [13]: First, the authors used a more probabilistic approach, based on Harris recurrence as developed by Meyn and Tweedie [11]. Second, a detailed analysis allowed them to understand the transfer of energy from the central oscillators to the (dissipative) baths. In that case the convergence to the stationary state is of exponential rate. In [1], this reasoning was extended to more general contexts.

The dynamics of the chain is very different when the pinning potential is *stronger* than the interaction potential. In that case the chain may have breathers, *i.e.*, oscillators concentrating a lot of energy, which is transferred only very slowly to their neighbours. This may lead to subexponential ergodicity, as shown by Hairer and Mattingly [8] in the case of a chain of 3 oscillators with strong pinning.

In this paper, we discuss a model with three rotors (see Figure 1), each given by an angle $q_i \in \mathbb{T} = \mathbb{R}/2\pi\mathbb{Z}$ and a momentum $p_i \in \mathbb{R}$, $i = 1, 2, 3$. The phase space is therefore $\Omega = \mathbb{T}^3 \times \mathbb{R}^3$, and we will consider the measure space (Ω, \mathcal{B}) , where \mathcal{B} is the Borel σ -field over Ω . We will denote the points of Ω by $x = (q, p)$ with $q = (q_1, q_2, q_3)$ and $p = (p_1, p_2, p_3)$.

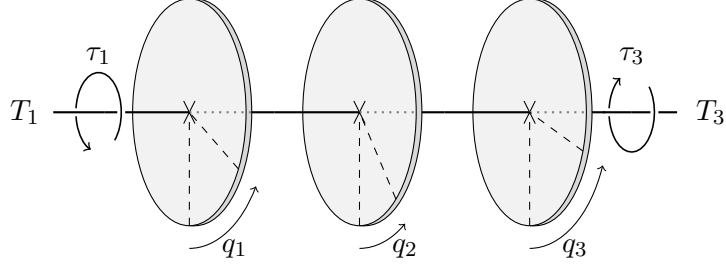


Figure 1 – A chain of three rotors with two external torques τ_1 and τ_3 and two heat baths at temperatures T_1 and T_3 .

We introduce the Hamiltonian

$$H(q, p) = \sum_{i=1}^3 \left(\frac{1}{2} p_i^2 + U_i(q_i) \right) + \sum_{b=1,3} W_b(q_2 - q_b),$$

with some smooth *interaction potentials* $W_b : \mathbb{T} \rightarrow \mathbb{R}$, $b = 1, 3$, and some smooth *pinning potentials* $U_i : \mathbb{T} \rightarrow \mathbb{R}$, $i = 1, 2, 3$. We now let the two outer rotors (*i.e.*, the rotors 1 and 3) interact with Langevin-type heat baths at temperatures $T_1, T_3 > 0$, and with coupling constants $\gamma_1, \gamma_3 > 0$. Moreover, we apply some constant (possibly zero) external forces τ_1 and τ_3 to the two outer rotors. Introducing $w_b = W'_b$ and $u_i = U'_i$, we obtain the system of SDE:

$$\begin{aligned} dq_i(t) &= p_i(t) dt, \quad i = 1, 2, 3, \\ dp_2(t) &= - \sum_{b=1,3} w_b(q_2(t) - q_b(t)) dt - u_2(q_2(t)) dt, \\ dp_b(t) &= \left(w_b(q_2(t) - q_b(t)) + \tau_b - u_b(q_b(t)) - \gamma_b p_b(t) \right) dt + \sqrt{2\gamma_b T_b} dB_t^b, \quad b = 1, 3, \end{aligned} \tag{1.1}$$

where B^1 and B^3 are standard independent Brownian motions.

Notation. In the sequel, the index b always refers to the rotors 1 and 3 at the boundaries of the chain, and we write \sum_b instead of $\sum_{b=1,3}$.

Remark 1.1. Our model can be viewed as an extreme case of that studied in [8]. A key factor in that paper is to realise how the frequency of one isolated pinned oscillator depends on its energy. Indeed, for an isolated oscillator with Hamiltonian $p^2/2 + q^{2k}/(2k)$, the frequency grows like the energy to the power $\frac{1}{2} - \frac{1}{2k}$. When $k \rightarrow \infty$, the exponent converges to $\frac{1}{2}$. In this limit, the pinning potential formally becomes an infinite potential well, so that the variable q is constrained to a compact interval. In our model, the position (angle) of a rotor lives in a compact space, and its frequency scales like its momentum, *i.e.*, like the square root of its energy. Therefore, we can view our rotor model as some kind of “infinite pinning” limit.

We make the following non-degeneracy assumption (clearly satisfied for *e.g.*, $w_1 = w_3 = \sin$):

Assumption 1.2. *There is at least one $b \in \{1, 3\}$ such that for each $s \in \mathbb{T}$, at least one of the derivatives $w_b^{(k)}(s)$, $k \geq 1$ is non-zero.*

For all initial conditions $x \in \Omega$ and all times $t \geq 0$, we denote by $P^t(x, \cdot)$ the transition probability of the Markov process associated to (1.1). Since the coefficients of the SDE (1.1) are globally Lipschitz, the solutions are almost surely defined for all times and all initial conditions, so that $P^t(x, \cdot)$ is well-defined as a probability measure on (Ω, \mathcal{B}) .

We now introduce the main theorem, in which we write

$$\|\nu\|_f = \sup_{|h| \leq f} \int_{\Omega} h d\nu$$

for any continuous function $f > 0$ on Ω and any signed measure ν on (Ω, \mathcal{B}) .

Theorem 1.3. *Under Assumption 1.2, the following holds for the Markov process defined by (1.1):*

- (i) *The transition kernel P^t has a density $p_t(x, y)$ in $C^\infty((0, \infty) \times \Omega \times \Omega)$.*
- (ii) *The process admits a unique invariant measure π , which has a smooth density.*
- (iii) *For all sufficiently small $\beta > 0$ and all $\beta' \in [0, \beta)$, there are constants $C, \lambda > 0$ such that for all $t \geq 0$ and all $x = (q_1, q_2, \dots, p_3) \in \Omega$,*

$$\|P^t(x, \cdot) - \pi\|_{e^{\beta'H}} \leq C(1 + p_2^2)e^{\beta H(x)}e^{-\lambda t^{1/2}}.$$

Remark 1.4. If both heat baths are at the same temperature, say, $T_1 = T_3 = T > 0$, and the forces τ_1 and τ_3 are zero, then the system is at thermal equilibrium and the Gibbs measure with density proportional to $e^{-H/T}$ is invariant. Indeed, one easily checks that this density verifies the stationary Fokker-Planck equation $L^*e^{-H/T} = 0$, where L^* is the formal adjoint of the generator L introduced below.

Remark 1.5. In fact, the results we prove here apply with hardly any modification to the “star” configuration with one central rotor interacting with m external rotors, which in turn are coupled to heat baths (*i.e.*, $m + 1$ rotors and m heat baths).

In addition, some studies (*e.g.*, [10]) consider chains with fixed boundary conditions. For the left end of the chain, this corresponds to adding a “dummy” rotor 0 which does not move but interacts with rotor 1. This is covered by our theory by adding some contribution to the pinning potential U_1 . The same applies to the right end and U_3 .

Chains of rotors provide toy models for the study of non-equilibrium statistical mechanics. In [10] long chains have been studied numerically, and it appears that even when the external temperatures are different and external forces are applied, local thermal equilibrium is satisfied in the stationary state in the limit of infinitely long chains. This stationary state may have some surprising features, like a large amount of energy in the bulk of the chain when the boundary conditions are properly chosen. In our case of course we are far from local thermal equilibrium, since we only study systems made of three rotors. We will present some numerical simulations of our system in §6, highlighting some interesting properties of the stationary state.

What corresponds here to the breathers observed in other models is the situation where the energy of the system is very large and mostly concentrated in the middle rotor. The middle rotor then spins very rapidly, and the interaction forces oscillate so fast that they have very little net effect. In this case, the middle rotor effectively decouples from the rest of the system, and the main difficulty is to show that its energy eventually decreases with some well-controlled bounds.

The idea used in [8] for the chain of three pinned oscillators is to average the oscillatory forces, and exhibit a negative feedback in the regime where the breather dominates the dynamics. The proof of Theorem 1.3 in the present paper is based on a systematisation of this idea, as explained in §3.4.

The paper is structured as follows: In §2 we introduce a sufficient condition for subgeometric ergodicity from [3]. In §3 we study the behaviour of the middle rotor. In §4 we show how to use the study of p_2 to get a Lyapunov function. In §5 we provide the necessary technical input to the theorem of [3]. Finally, we illustrate numerically some properties of the non-equilibrium steady state in §6.

2 Ergodicity and Lyapunov functions

The proof of Theorem 1.3 relies on the results of [3] which in turn are based on the theory exposed in [11]. The theory of [11] shows that one can prove the ergodicity of an irreducible Markov process and estimate the rate of convergence toward its invariant measure if one has a good control of the return times of the process to particular sets, called *petite sets*. A set K is petite if there exist a probability measure a on $[0, \infty)$ and a non-zero measure ν_a on Ω such that for all $x \in K$ one has $\int_0^\infty P^t(x, \cdot) a(dt) \geq \nu_a(\cdot)$. In the case we are interested in, control arguments and the hypoellipticity of the generator imply that each compact set is petite (see §5.1 for a proof of this property).

Let L be the infinitesimal generator of the process, *i.e.*, the second-order differential operator

$$L = \sum_{i=1}^3 (p_i \partial_{q_i} - u_i(q_i) \partial_{p_i}) + \sum_b [w_b(q_2 - q_b)(\partial_{p_b} - \partial_{p_2}) + \tau_b \partial_{p_b} - \gamma_b p_b \partial_{p_b} + \gamma_b T_b \partial_{p_b}^2] .$$

Recall that for any sufficiently regular function f we have $Lf(x) = \frac{d}{dt} [\int f(y) P_t(x, dy)]|_{t=0}$.

A classical way to control the return times to a petite set is to make use of Lyapunov functions. We call *Lyapunov function* a smooth function $V : \Omega \mapsto [1, \infty)$ with compact level sets (*i.e.*, due to the structure of Ω , a function such that $V(q, p) \rightarrow \infty$ when $\|p\| \rightarrow \infty$) such that for all $x \in \Omega$,

$$(LV)(x) \leq C \mathbf{1}_K(x) - \varphi \circ V(x) , \quad (2.1)$$

where C is a constant, $\varphi : [1, \infty) \rightarrow (0, \infty)$ is an increasing function, and K is a petite set. If one can find such a function, and prove that some skeleton $P^\Delta(\Delta > 0)$ is μ -irreducible for some measure μ (*i.e.*, $\mu(A) > 0$ implies that for all $x \in \Omega$ there exists $k \in \mathbb{N}$ such that $P^{k\Delta}(x, A) > 0$), then the Markov process is ergodic, with rate depending on φ . In the case where $\varphi(V) \propto V^\varrho$, the convergence is geometric if $\varrho = 1$ and polynomial if $\varrho < 1$ (see [3, 12]). In this paper, we obtain $\varphi(V) \sim V/\log V$.

We rely on the work of Douc, Fort and Guillin [3], which gives a sufficient condition for subgeometric ergodicity of continuous-time Markov processes. We give here a simplified version of their result, adapted to our purpose. This statement is based on Theorem 3.2 and Theorem 3.4 of [3].

Theorem 2.1 (Douc-Fort-Guillin (2009)). *Assume that the process has an irreducible skeleton and that there exist a smooth function $V : \Omega \rightarrow [1, \infty)$ with $V(q, p) \rightarrow \infty$ when $\|p\| \rightarrow \infty$, an increasing, differentiable, concave function $\varphi : [1, \infty) \rightarrow (0, \infty)$, a petite set K , and a constant C such that (2.1) holds. Then the process admits a unique invariant measure π , and for each $z \in [0, 1]$, there exists a constant C' such that for all $t \geq 0$ and all $x \in \Omega$,*

$$\|P^t(x, \cdot) - \pi\|_{(\varphi \circ V)^z} \leq g(t) C' V(x) ,$$

where $g(t) = (\varphi \circ H_\varphi^{-1}(t))^{z-1}$, with $H_\varphi(u) = \int_1^u \frac{ds}{\varphi(s)}$.

When $z = 0$, we retrieve the total variation norm $\|P^t(x, \cdot) - \pi\|_{TV}$ and the rate is the fastest. Increasing z strengthens the norm but slows the convergence rate down. When $z = 1$, the norm is the strongest, but no convergence is guaranteed since $g(t) \equiv 1$.

The core of the paper is devoted to the construction of a Lyapunov function such that (2.1) is satisfied with $\varphi(s) \sim s/\log s$, and a set K which is compact and therefore petite. This yields a stretched exponential convergence rate (see (2.4)). The existence of an irreducible skeleton required by Theorem 2.1 and the fact that every compact set is petite are proved in §5.

One might at first think that a Lyapunov function is simply given by the Hamiltonian H . Unfortunately, this is not the case, as

$$LH = \sum_b (\tau_b p_b + \gamma_b (T_b - p_b^2)) , \quad (2.2)$$

where the right-hand side remains positive when p_1, p_3 are small and $p_2 \rightarrow \infty$. Thus, there is no bound of the form (2.1) for H . The same problem occurs if we take any function $f(H)$ of the energy.

In order to find a *bona fide* Lyapunov function, we will need more insight into how fast all *three* momenta decrease. The equality (2.2) suggests that p_1 and p_3 will not cause any problem. In fact, we have for $b = 1, 3$, that

$$Lp_b = -\gamma_b p_b + w_b(q_2 - q_b) - u_b(q_b) + \tau_b .$$

Since $w_b(q_2 - q_b) - u_b(q_b) + \tau_b$ is bounded, $|p_b|$ essentially decays at exponential rate when it is large. This is of course due to the friction terms that act on p_1 and p_3 directly. Such a result does not hold for p_2 . In fact, the decay of p_2 is much slower. Our main insight is that in a sense

$$Lp_2 \sim -cp_2^{-3} .$$

The proof of such a relation occupies a major part of this paper. As indicated earlier, this very slow damping of p_2 comes from the lack of effective interaction when the forces oscillate very rapidly. Once we have gained enough understanding of the dynamics of p_2 , we will be able to construct a Lyapunov function, whose properties are summarised in

Proposition 2.2. *For all sufficiently small $\beta > 0$, there is a function $V : \Omega \rightarrow [1, \infty)$ satisfying the two following properties:*

1. *There are positive constants c_1, c_2 such that*

$$1 + c_1 e^{\beta H} \leq V \leq c_2 (1 + p_2^2) e^{\beta H} .$$

2. *There are positive constants c_3, c_4 and a compact set K such that*

$$LV \leq c_3 \mathbf{1}_K - \varphi(V) ,$$

where $\varphi : [1, \infty) \rightarrow (0, \infty)$ is defined by¹

$$\varphi(s) = \frac{c_4 s}{2 + \log(s)} . \quad (2.3)$$

The way we construct the Lyapunov function is somewhat different from that of [8]. There, it is obtained starting from some power of the Hamiltonian and then adding corrections by an averaging technique similar to ours (see Remark 3.8). Here, we first average the dynamics of p_2 and then use the result to construct a Lyapunov function that essentially grows exponentially with the energy. This gives a stretched exponential rate of convergence instead of a polynomial rate as in [8]. The present method can in principle be applied to the model of [8] (see also [7]).

We now show how the main results follows.

Proof of Theorem 1.3. The conclusions of Theorem 1.3 immediately follow from Theorem 2.1, Proposition 2.2, the technical results stated in Proposition 5.1, and the following two observations. Consider $0 \leq \beta' < \beta$ and choose $z \in (0, 1)$ such that $\beta' < z\beta$. First, the function φ defined in (2.3) yields, in the notation of Theorem 2.1, a convergence rate

$$g(t) = (\varphi \circ H_\varphi^{-1}(t))^{z-1} \leq ce^{-\lambda t^{1/2}} \quad (2.4)$$

for some $c, \lambda > 0$. Indeed, we have $H_\varphi(u) = \frac{1}{c_4} \int_1^u \frac{2+\log s}{s} ds = \frac{1}{2c_4} (\log u)^2 + \frac{2}{c_4} \log u$, so that $H_\varphi^{-1}(t) = \exp((2c_4 t + 4)^{1/2} - 2)$ and $(\varphi \circ H_\varphi^{-1}(t)) = (2c_4 t + 4)^{-1/2} \exp((2c_4 t + 4)^{1/2} - 2) \geq Ce^{C't^{1/2}}$ for some $C, C' > 0$. Thus, (2.4) holds with $\lambda = (1 - z)C'$. Secondly, by Proposition 2.2 (i), and since $\beta' < z\beta$, we observe that $e^{\beta' H} \leq c(\varphi \circ V)^z$ for some constant $c > 0$, so that $\|\cdot\|_{e^{\beta' H}} \leq c \|\cdot\|_{(\varphi \circ V)^z}$. \square

¹The 2 in the denominator ensures that φ is concave and increasing on $[1, \infty)$, as required in Theorem 2.1.

3 Effective dynamics for the middle rotor

The hardest and most interesting part of the problem is to determine how p_2 decreases when it is very large.² In this section, we obtain some asymptotic, effective dynamics for p_2 when $p_2 \rightarrow \infty$.

3.1 Expected rate

Before we start making any proof, we can get a hint of how p_2 decreases in the regime where p_2 is very large and both p_1, p_3 are small. Assume for simplicity that $u_i \equiv 0$ and that $W_b(s) = -\varkappa \cos(s)$ so that $w_b(s) = \varkappa \sin(s)$. In the regime of interest, we expect the middle rotor to decouple, so that p_2 will evolve very slowly. We will consider the system over times that are small enough for p_2 to remain almost constant (say equal to ω), but large enough for some “quasi-stationary” regime to be reached. The reader can think of ω as being the “initial” value of p_2 . For $b = 1, 3$, we expect p_b to be well approximated, at least qualitatively, by the equation

$$dp_b = \varkappa \sin(\omega t) dt - \gamma_b p_b dt + \sqrt{2\gamma_b T_b} dB_t^b,$$

whose solution is

$$\begin{aligned} p_b(t) &= \varkappa \frac{\gamma_b \sin(\omega t) - \omega \cos(\omega t)}{\gamma_b^2 + \omega^2} + \sqrt{2\gamma_b T_b} \int_0^t e^{\gamma_b(s-t)} dB_s^b \\ &= -\varkappa \frac{\cos(\omega t)}{\omega} + \sqrt{2\gamma_b T_b} \int_0^t e^{\gamma_b(s-t)} dB_s^b + \mathcal{O}\left(\frac{1}{\omega^2}\right). \end{aligned}$$

We have neglected the exponentially decaying part $p_b(0)e^{-\gamma_b t}$ since we assume that a quasi-stationary regime is reached. By (2.2), the rate of energy flowing *into* of the system at b is $\gamma_b(T_b - p_b^2)$. Squaring p_b and taking expectations, what remains is

$$\begin{aligned} \mathbb{E}p_b^2(t) &= \varkappa^2 \frac{\cos^2(\omega t)}{\omega^2} + 2\gamma_b T_b \mathbb{E} \left(\int_0^t e^{\gamma_b(s-t)} dB_s^b \right)^2 + \mathcal{O}\left(\frac{1}{\omega^3}\right) \\ &= \varkappa^2 \frac{\cos^2(\omega t)}{\omega^2} + (1 - e^{-2\gamma_b t})T_b + \mathcal{O}\left(\frac{1}{\omega^3}\right), \end{aligned}$$

where we have used the Itô isometry $\mathbb{E}(\int_0^t e^{\gamma_b(s-t)} dB_s^b)^2 = \int_0^t e^{2\gamma_b(s-t)} ds$. Neglecting again an exponentially decaying term, we obtain

$$\frac{d}{dt} \mathbb{E}H(t) = \sum_b \mathbb{E}(\gamma_b(T_b - p_b^2(t))) \sim - \sum_b \gamma_b \varkappa^2 \frac{\cos^2(\omega t)}{\omega^2}. \quad (3.1)$$

Since $\cos^2(\omega t)$ oscillates very rapidly around its average $1/2$, we expect to see an effective contribution $-\frac{\gamma_b \varkappa^2}{2\omega^2}$. This approximation was obtained by assuming that p_2 is almost constant and equal to ω . Now, when p_2 is very large, the energy H is dominated by the contribution $\frac{1}{2}p_2^2$, so that we expect to have $\frac{d}{dt} \mathbb{E}H \sim p_2 \frac{d}{dt} \mathbb{E}p_2$. Comparison with (3.1) leads to

$$\frac{d}{dt} \mathbb{E}p_2 \sim -\frac{1}{p_2^3} \sum_b \frac{\gamma_b \varkappa^2}{2}.$$

We will obtain this result rigorously in Proposition 3.4.

²To simplify notation, we say p_2 is large, but we always really mean that $|p_2|$ is large.

3.2 Notations

Let $\Omega^\dagger = \{(q, p) \in \Omega : p_2 \neq 0\}$. We denote throughout by $X_t = (q(t), p(t))$ the solution of the stochastic differential equation (1.1) with initial condition $X_0 = (q(0), p(0))$. For now, we restrict ourselves to $X_0 \in \Omega^\dagger$ since we aim to obtain an effective dynamics for the middle rotor by performing an expansion in negative powers of p_2 . Remark that since $\frac{d}{dt}p_2$ is bounded, there is for each initial condition $X_0 \in \Omega^\dagger$ a deterministic time $t^* > 0$ (proportional to $|p_2(0)|$) such that $X_t \in \Omega^\dagger$ for all $t \in [0, t^*)$ and all realisations of the random noises. To define a smooth Lyapunov function on the whole space Ω we will perform a regularisation in §4.

Definition 3.1. We let \mathcal{U} be the set of stochastic processes u_t which are solutions of an SDE of the form

$$du_t = f_1(X_t)dt + f_2(X_t)dB_t^1 + f_3(X_t)dB_t^3, \quad (3.2)$$

for some functions $f_i : \Omega \rightarrow \mathbb{R}$.

Notation: In the sequel, we write

$$du_t = f_1 dt + f_2 dB_t^1 + f_3 dB_t^3$$

instead of (3.2).

For any smooth function h on Ω , the stochastic process $h(X_t)$ is in \mathcal{U} by the Itô formula (see below). Without further mention, we will both see h as a function on Ω and as the stochastic process $h(X_t)$. When referring to the stochastic process, we shall write simply dh instead of $dh(X_t)$. Of course, only very few processes in \mathcal{U} can be written in the form $h(X_t)$ for some function h on Ω .

The variables p_2 and q_2 will play a special role, as we are merely interested in the regime where p_2 is very large. For any function f over Ω we call the quantity

$$\langle f \rangle = \frac{1}{2\pi} \int_0^{2\pi} f dq_2$$

the q_2 -average of f (or simply the average of f), which is a function of p, q_1 and q_3 only.

Assumption 3.2. We assume

$$\langle U_2 \rangle = 0 \quad \text{and} \quad \langle W_b \rangle = 0, \quad b = 1, 3.$$

This assumption merely fixes the additive constants of the potentials and therefore results in no loss of generality.

For conciseness, we shall omit the arguments of the potentials and forces, always assuming that

$$\begin{aligned} W_b &= W_b(q_2 - q_b), & w_b &= w_b(q_2 - q_b), & b &= 1, 3, \\ U_i &= U_i(q_i), & u_i &= u_i(q_i), & i &= 1, 2, 3. \end{aligned}$$

To simplify the notations, we also introduce the potentials Φ_1, Φ_2, Φ_3 associated to the three rotors, and the corresponding forces $\varphi_1, \varphi_2, \varphi_3$ defined by

$$\begin{aligned} \Phi_b &= W_b + U_b, & \varphi_b &= -\partial_{q_b} \Phi_b = w_b - u_b, & b &= 1, 3, \\ \Phi_2 &= W_1 + W_3 + U_2, & \varphi_2 &= -\partial_{q_2} \Phi_2 = -w_1 - w_3 - u_2. \end{aligned} \quad (3.3)$$

Of course, Φ_i and φ_i are functions of q only. With these notations the dynamics reads more concisely

$$\begin{aligned} dq_i &= p_i dt, & i &= 1, 2, 3, \\ dp_2 &= \varphi_2 dt, \\ dp_b &= \left(\varphi_b + \tau_b - \gamma_b p_b \right) dt + \sqrt{2\gamma_b T_b} dB_t^b, & b &= 1, 3. \end{aligned}$$

We will mainly deal with functions of the form $p_2^\ell p_1^n p_3^m g(q)$ and their linear combinations. We therefore introduce the notion of degree.

Definition 3.3. We say that a function f on Ω^\dagger has degree $\ell \in \mathbb{Z}$ if it can be written as a finite sum of elements of the kind $p_2^\ell p_1^n p_3^m g(q)$ for some $n, m \in \mathbb{N}$ and a smooth function $g : \mathbb{T}^3 \rightarrow \mathbb{R}$. Moreover, we denote

$$\hat{\mathcal{O}}(p_2^\ell)$$

a generic expression of order at most ℓ (which can vary from line to line), i.e., a finite sum of functions of degree $\ell, \ell - 1, \ell - 2, \dots$.

We have by the Itô formula that for any smooth function f on Ω

$$\begin{aligned} df &= \sum_{i=1}^3 \left(\frac{\partial f}{\partial q_i} dq_i + \frac{\partial f}{\partial p_i} dp_i \right) + \sum_b \gamma_b T_b \frac{\partial^2 f}{\partial p_b^2} dt \\ &= d^+ f + d^0 f + d^- f, \end{aligned}$$

where

$$\begin{aligned} d^+ f &= p_2 \frac{\partial f}{\partial q_2} dt, \\ d^- f &= \varphi_2 \frac{\partial f}{\partial p_2} dt, \\ d^0 f &= \sum_b \left(p_b \frac{\partial f}{\partial q_b} + (\varphi_b + \tau_b - \gamma_b p_b) \frac{\partial f}{\partial p_b} + \gamma_b T_b \frac{\partial^2 f}{\partial p_b^2} \right) dt + \sum_b \sqrt{2\gamma_b T_b} \frac{\partial f}{\partial p_b} dB_t^b. \end{aligned} \tag{3.4}$$

(By the discussion following Definition 3.1, f , its partial derivatives, p_2 and the functions φ_i in this SDE are evaluated on the trajectory X_t .) Observe that when acting on a function of degree ℓ , the contribution d^+ increases the degree of p_2 by one, while d^0 and d^- respectively leave it unchanged and decrease it by one. In this sense, we will see d^+ as the “dominant” part of d .

3.3 General idea

In this section we introduce the main idea, which consists in successively removing oscillatory terms order by order in the dynamics of p_2 . We perform here the first step of the method in a somewhat naive, but pedestrian way. In the next two sections, we systematise the method and apply it.

We begin by looking at the equation

$$dp_2 = \varphi_2 dt. \tag{3.5}$$

When p_2 is large while p_1 and p_3 are small, the right-hand side is highly oscillatory and its time-average is almost zero, since $\langle \varphi_2 \rangle = 0$. We will proceed to a change of variable in order to “see through” this oscillatory term.

We first make the relation between the time-average and the q_2 -average more precise. Consider some function g on Ω . In the regime where p_2 is very large and p_1, p_3 are small, the only fast variable is q_2 . Now consider some interval of time $[0, T]$ short enough so that the other variables do not change significantly, but still large enough for q_2 to swipe through $[0, 2\pi)$ many times. We have in that case $q_2(t) \sim q_2(0) + p_2(0)t$ (remember that q_2 is defined modulo 2π) and

$$g(q(t), p(t)) \sim g(q_1(0), q_2(0) + p_2(0)t, q_3(0), p(0)), \tag{3.6}$$

so that the time-average of g is expected to be very close to the q_2 -average $\langle g \rangle$.

Now, we want to estimate $p_2(t) = \int_0^t \varphi_2(q(s)) ds$ in this situation. Approximating φ_2 as in (3.6) and integrating formally with respect to time (remember that $\varphi_2 = -\partial_{q_2} \Phi_2$) leads naturally to the decomposition

$$p_2 = \bar{p}_2 - \frac{\Phi_2(q)}{p_2}, \tag{3.7}$$

which consists in writing p_2 as sum of an oscillatory term Φ_2/p_2 which is supposed to capture “most” of the oscillatory dynamics, and some (hopefully) nicely behaved “slow” process \bar{p}_2 . And indeed, if we differentiate (3.7) we get

$$\begin{aligned}
d\bar{p}_2 &= d\left(p_2 + \frac{\Phi_2}{p_2}\right) \\
&= dp_2 + d^+\frac{\Phi_2}{p_2} + d^0\frac{\Phi_2}{p_2} + d^-\frac{\Phi_2}{p_2} \\
&= \varphi_2 dt - \varphi_2 dt - \left(\frac{p_1 w_1}{p_2} + \frac{p_3 w_3}{p_2}\right) dt - \frac{\varphi_2 \Phi_2}{p_2^2} dt \\
&= -\left(\frac{p_1 w_1}{p_2} + \frac{p_3 w_3}{p_2}\right) dt - \frac{\varphi_2 \Phi_2}{p_2^2} dt .
\end{aligned} \tag{3.8}$$

As a result, we have a new process \bar{p}_2 which is asymptotically equal to p_2 in the regime of interest, and whose dynamics involves only terms that are small when p_2 is large, so that \bar{p}_2 is indeed a slow variable. Observe that the choice of adding Φ_2/p_2 to p_2 has the effect that $d^+(\Phi_2/p_2) = -\varphi_2 dt$, which precisely cancels the right-hand side of (3.5) while the remaining terms have negative powers of p_2 . This observation is the starting point of the systematisation of the method.

Unfortunately, (3.8) is not good enough to understand how \bar{p}_2 (and therefore p_2) decreases in the long run, since the dynamics (3.8) of \bar{p}_2 still involves oscillatory terms. The idea is therefore to eliminate these oscillatory terms by absorbing them into a further change of variable $\bar{p}_2 = \bar{\bar{p}}_2 + G$ for some suitably chosen G . The result is that $d\bar{\bar{p}}_2$ is a sum of terms of degree -2 at most, which turn out to be still oscillatory. This procedure must then be iterated, successively eliminating oscillatory terms order by order, until we get some dynamics that has a non-zero average (which happens after finitely many steps). We will follow this idea, but in a way that does not require to write the successive changes of variable explicitly. More precisely, we will prove

Proposition 3.4. *There is a function $F = \frac{\Phi_2(q)}{p_2} + \hat{O}(p_2^{-2})$ such that whenever $p_2(t) \neq 0$ the process $\tilde{p}_2(t) = p_2(t) + F(X_t)$ satisfies*

$$d\tilde{p}_2(t) = a(X_t) dt + \sum_b \sigma_b(X_t) dB_t^b , \tag{3.9}$$

with

$$\begin{aligned}
a(q, p) &= -\frac{\gamma_1 \langle W_1^2 \rangle + \gamma_3 \langle W_3^2 \rangle}{p_2^3} + \hat{O}(p_2^{-4}) , \\
\sigma_b(q, p) &= \frac{\sqrt{2\gamma_b T_b} W_b}{p_2^2} + \hat{O}(p_2^{-3}) , \quad b = 1, 3 .
\end{aligned}$$

(By Assumption 3.2, no arbitrary additive constant appears in $\langle W_1^2 \rangle$ and $\langle W_3^2 \rangle$.)

The next two sections are devoted to proving Proposition 3.4.

3.4 Averaging

The crux of our analysis is to average oscillatory terms in the dynamics. This is a well known problem in differential equations. In classical averaging theory [14, 16], it is an *external* small parameter ε that gives the time scale of the fast variables. Here, the role of ε is played by $1/p_2$, which is a dynamical variable. We develop an averaging theory adapted to this case, and also to the stochastic nature of the problem.

The starting point is as follows. Imagine that for a function h on Ω we find an expression of the kind

$$dh = f dt + dr_t , \tag{3.10}$$

for some function $f = f(X_t)$ of degree ℓ and some stochastic process $r_t \in \mathcal{U}$ (see Definition 3.1) which denotes the part of the dynamics that we do not want to interfere with. Thinking of $f(X_t)$ as a highly oscillatory quantity when p_2 is very large, we would like to write $h = \bar{h} + F$ for some small function F on Ω such that

$$d\bar{h} = \langle f \rangle dt + dr_t + \text{small corrections} , \quad (3.11)$$

where the notion of *small* will be made precise in terms of powers of p_2 . That is, we want to find some \bar{h} close to h , such that its dynamics involves, instead of $f dt$, the q_2 -average $\langle f \rangle dt$ plus some smaller corrections. In other words, we are looking for some F such that

$$dF = d(h - \bar{h}) = (f - \langle f \rangle) dt + \text{small corrections} .$$

Remembering that in terms of powers of p_2 , d^+ is the dominant part of d , the key is to find some F such that $d^+ F = (f - \langle f \rangle) dt$. If we write $L^+ = p_2 \partial_{q_2}$, we have $d^+ F = L^+ F dt$. Thus, we really need to invert L^+ (which is in fact the dominant part of the generator L when p_2 is large).

We call here \mathcal{K} the space of smooth functions $\Omega^\dagger \rightarrow \mathbb{R}$, and we denote by \mathcal{K}_0 the space of functions $f \in \mathcal{K}$ such that $\langle f \rangle = 0$. Note that L^+ maps \mathcal{K} to \mathcal{K}_0 since for all $f \in \mathcal{K}$, we have by periodicity

$$\langle L^+ f \rangle = p_2 \langle \partial_{q_2} f \rangle = 0 .$$

We can define a right inverse $(L^+)^{-1} : \mathcal{K}_0 \rightarrow \mathcal{K}_0$ by letting for all $g \in \mathcal{K}_0$

$$(L^+)^{-1} g = \frac{1}{p_2} \left(\int g dq_2 + c(p, q_1, q_3) \right) ,$$

where the integration “constant” $c(p, q_1, q_3)$ is uniquely defined by requiring that $\langle (L^+)^{-1} g \rangle = 0$.

This leads naturally to the following

Definition 3.5. For any function $f \in \mathcal{K}$, we define the operator $Q : \mathcal{K} \rightarrow \mathcal{K}_0$ by

$$Qf = (L^+)^{-1} (f - \langle f \rangle) .$$

Remark 3.6.

- If f is a function of degree ℓ , then Qf is of degree $\ell - 1$.
- By construction,

$$d(Qf) = (f - \langle f \rangle) dt + d^0(Qf) + d^-(Qf) . \quad (3.12)$$

- Moreover, by definition, Qf is the only function such that

$$\partial_{q_2}(Qf) = \frac{f - \langle f \rangle}{p_2} \quad \text{and} \quad \langle Qf \rangle = 0 . \quad (3.13)$$

Therefore, if (3.10) holds for some f of degree ℓ , then we obtain a quantitative expression for (3.11), namely

$$d(h - Qf) = \langle f \rangle dt + dr_t - d^0(Qf) - d^-(Qf) ,$$

where the corrections are small in the sense that Qf , $d^0(Qf)$ and $d^-(Qf)$ have degree respectively $\ell - 1$, $\ell - 1$ and $\ell - 2$.

Remark 3.7. Observe that (3.7) can be written now as $p_2 = \bar{p}_2 + Q\varphi_2$, since $Q\varphi_2 = -\Phi_2/p_2$. Thus, the “naive” correction we added in (3.7) also follows from the systematic method we have just introduced. This is no surprise: the naive correction in (3.7) was motivated by the approximation (3.6) in which only q_2 moves, which corresponds to considering only d^+ .

Remark 3.8. Our averaging procedure is inspired by techniques of [8]. There, the equivalent of L^+ is the generator $-q_2^{2k-1}\partial_{p_2} + p_2\partial_{q_2}$ of the free dynamics of the middle oscillator, where $q_2^{2k}/(2k)$ is the pinning potential. In their case, one cannot explicitly invert L^+ , but one can show that $(L^+)^{-1}$ basically acts as a division by $E_2^{\frac{1}{2}-\frac{1}{2k}}$, where E_2 is the energy of the middle oscillator. Again, taking formally the limit $k \rightarrow \infty$, one obtains that $(L^+)^{-1}$ acts as a division by $\sqrt{E_2}$, much like in our case where $(L^+)^{-1}$ acts as a division by $p_2 \sim \sqrt{E_2}$.

We now restate our averaging method as the following lemma, which follows from a trivial rearrangement of the terms in (3.12).

Lemma 3.9. (*Averaging lemma*) Consider some function $f = \hat{O}(p_2^\ell)$ for some $\ell \in \mathbb{Z}$. Then

$$f \, dt = \langle f \rangle \, dt - d^0(Qf) - d^-(Qf) + d(Qf) ,$$

where $d^0(Qf)$ is of degree $\ell - 1$ at most and $d^-(Qf)$ is of degree $\ell - 2$ at most.

We now prove Proposition 3.4 by using Lemma 3.9 repeatedly.

3.5 Proof of Proposition 3.4

We make the following observations, which we will use without reference. For any function f on Ω^\dagger that is smooth in q_2 , we have by periodicity

$$\langle \partial_{q_2} f \rangle = 0 . \quad (3.14)$$

Moreover, if g is another such function, then we can integrate by parts to obtain

$$\langle (\partial_{q_2} f) g \rangle = - \langle f \partial_{q_2} g \rangle .$$

Furthermore, we have by Assumption 3.2, (3.3) and (3.14) that

$$\langle W_b \rangle = \langle w_b \rangle = \langle \Phi_2 \rangle = \langle \varphi_2 \rangle = 0 .$$

We start by doing again the first step, which we did in §3.3, but this time using the new toolset. In order to average the right-hand side of

$$dp_2 = \varphi_2 \, dt ,$$

we use Lemma 3.9 with $f = \varphi_2$, which is of order 0. We have $\langle f \rangle = 0$ and $Qf = -\Phi_2/p_2$ (by definition of φ_2 and Φ_2). We obtain

$$\begin{aligned} dp_2 &= d^0\left(\frac{\Phi_2}{p_2}\right) + d^-\left(\frac{\Phi_2}{p_2}\right) - d\left(\frac{\Phi_2}{p_2}\right) \\ &= \frac{1}{p_2} \sum_b p_b \frac{\partial \Phi_2}{\partial q_b} \, dt - \frac{\varphi_2 \Phi_2}{p_2^2} \, dt - d\left(\frac{\Phi_2}{p_2}\right) \\ &= -\frac{1}{p_2} \sum_b p_b w_b \, dt - \frac{\varphi_2 \Phi_2}{p_2^2} \, dt - d\left(\frac{\Phi_2}{p_2}\right) . \end{aligned} \quad (3.15)$$

This is exactly what we found in (3.8). We deal next with the terms $-p_b w_b/p_2 \, dt$ in (3.15). Using Lemma 3.9 with $f = p_b w_b/p_2$ (and therefore with $Qf = p_b W_b/p_2^2$), we find, since $\langle f \rangle = p_b \langle w_b \rangle / p_2 = 0$, that for $b = 1, 3$,

$$\begin{aligned} \frac{p_b w_b}{p_2} \, dt &= -\frac{1}{p_2^2} [-p_b^2 w_b + (\varphi_b + \tau_b - \gamma_b p_b) W_b] \, dt \\ &\quad - \frac{1}{p_2^2} \sqrt{2\gamma_b T_b} W_b dB_t^b + \frac{2}{p_2^3} p_b W_b \varphi_2 \, dt + d\hat{O}(p_2^{-2}) , \end{aligned} \quad (3.16)$$

where here and in the sequel, we denote by $d\hat{O}(p_2^k)$ any generic expression of the kind $dw(X_t)$ for some function $w = \hat{O}(p_2^k)$ on Ω . Here $d\hat{O}(p_2^{-2}) = d(p_b W_b p_2^{-2})$. Substituting (3.16) into (3.15) leads to

$$dp_2 = I dt + J dt + \frac{1}{p_2^2} \sum_b \sqrt{2\gamma_b T_b} W_b dB_t^b + d\left(-\frac{\Phi_2}{p_2} + \hat{O}(p_2^{-2})\right), \quad (3.17)$$

with

$$I = - \sum_b \frac{p_b^2 w_b - (\varphi_b + \tau_b - \gamma_b p_b) W_b}{p_2^2} - \frac{\varphi_2 \Phi_2}{p_2^2},$$

$$J = \frac{2}{p_2^3} \sum_b p_b W_b \varphi_2.$$

We next deal with the terms $I dt$ and $J dt$.

First, we show that $\langle I \rangle = 0$. It is immediate that $\langle p_2^{-2} p_b^2 w_b \rangle$ and $\langle p_2^{-2} (\tau_b - \gamma_b p_b) W_b \rangle$ are zero. Moreover, $\langle p_2^{-2} \varphi_2 \Phi_2 \rangle = -\frac{1}{2} p_2^{-2} \langle \partial_{q_2} \Phi_2^2 \rangle = 0$. Thus,

$$\begin{aligned} \langle I \rangle &= \sum_b \left\langle \frac{1}{p_2^2} \varphi_b W_b \right\rangle = \sum_b \left\langle \frac{w_b - u_b}{p_2^2} W_b \right\rangle \\ &= - \sum_b \left(\frac{\langle \partial_{q_2} W_b^2 \rangle}{2p_2^2} + \frac{u_b \langle W_b \rangle}{p_2^2} \right) = 0. \end{aligned}$$

Since I is of order -2 and $\langle I \rangle = 0$, we find that QI is of order -3 and thus $d^-(QI) = \hat{O}(p_2^{-4}) dt$. Applying Lemma 3.9 with $f = I$, we find

$$I dt = -d^0(QI) + \hat{O}(p_2^{-4}) dt + d\hat{O}(p_2^{-3}). \quad (3.18)$$

Using that $\langle QI \rangle = 0$, the definition (3.4) of d^0 leads, upon inspection, to

$$d^0(QI) = \sum_b w_b \partial_{p_b}(QI) dt + \mathcal{E} dt + \sum_b \hat{O}(p_2^{-3}) dB_t^b,$$

where \mathcal{E} is a sum of terms of order -3 and $\langle \mathcal{E} \rangle = 0$. Applying Lemma 3.9 to $w_b \partial_{p_b}(QI) dt$ and $\mathcal{E} dt$, we obtain

$$d^0(QI) = \sum_b \langle w_b \partial_{p_b}(QI) \rangle dt + \hat{O}(p_2^{-4}) dt + \sum_b \hat{O}(p_2^{-3}) dB_t^b. \quad (3.19)$$

Using the definition of w_b , integrating by parts once and using (3.13), we have for $b = 1, 3$,

$$\langle w_b \partial_{p_b}(QI) \rangle = \langle \partial_{q_2}(W_b) Q(\partial_{p_b} I) \rangle = -\langle W_b \partial_{q_2} Q(\partial_{p_b} I) \rangle = -\frac{1}{p_2} \langle W_b \partial_{p_b} I \rangle.$$

Since $\partial_{p_b} I = -p_2^{-2} (2p_b w_b + \gamma_b W_b)$, we get

$$\langle w_b \partial_{p_b}(QI) \rangle = \left\langle \frac{1}{p_2^3} W_b (2p_b w_b + \gamma_b W_b) \right\rangle = \frac{1}{p_2^3} \gamma_b \langle W_b^2 \rangle, \quad (3.20)$$

where again we have used that $\langle W_b w_b \rangle = \frac{1}{2} \langle \partial_{q_2} W_b^2 \rangle = 0$. Substituting (3.20) into (3.19) and then the result into (3.18) we finally get

$$I dt = -\frac{\alpha}{p_2^3} dt + \sum_b \hat{O}(p_2^{-3}) dB_t^b + \hat{O}(p_2^{-4}) dt + d\hat{O}(p_2^{-3}), \quad (3.21)$$

where

$$\alpha = \sum_b \gamma_b \langle W_b^2 \rangle .$$

We next deal with the term $J dt$ of (3.17). First, by Lemma 3.9,

$$J dt = \langle J \rangle dt + \hat{O}(p_2^{-4}) dt + \sum_b \hat{O}(p_2^{-4}) dB_t^b + d\hat{O}(p_2^{-4}) . \quad (3.22)$$

Unfortunately, $\langle J \rangle \neq 0$,³ and we will need some more subtle identifications. Integrating by parts, we have

$$\begin{aligned} \langle J \rangle &= \frac{2p_b}{p_2^3} \sum_b \langle W_b \varphi_2 \rangle = -\frac{2p_b}{p_2^3} \sum_b \langle W_b \partial_{q_2} \Phi_2 \rangle \\ &= \frac{2p_b}{p_2^3} \sum_b \langle (\partial_{q_2} W_b) \Phi_2 \rangle = \frac{2p_b}{p_2^3} \sum_b \langle w_b \Phi_2 \rangle \\ &= -\frac{1}{p_2^3} \sum_b p_b \partial_{q_b} \langle \Phi_2^2 \rangle . \end{aligned} \quad (3.23)$$

On the other hand, since $p_2^{-3} \langle \Phi_2^2 \rangle$ does not depend on q_2 , we find $d^+(p_2^{-3} \langle \Phi_2^2 \rangle) = 0$, so that

$$\begin{aligned} d \left(\frac{\langle \Phi_2^2 \rangle}{p_2^3} \right) &= d^0 \left(\frac{\langle \Phi_2^2 \rangle}{p_2^3} \right) + d^- \left(\frac{\langle \Phi_2^2 \rangle}{p_2^3} \right) \\ &= \sum_b p_b \partial_{q_b} \left(\frac{\langle \Phi_2^2 \rangle}{p_2^3} \right) dt + \hat{O}(p_2^{-4}) dt . \end{aligned} \quad (3.24)$$

Combining (3.23) and (3.24) we find

$$\langle J \rangle dt = \hat{O}(p_2^{-4}) dt + d(p_2^{-3} \langle \Phi_2^2 \rangle) = \hat{O}(p_2^{-4}) dt + d\hat{O}(p_2^{-3}) ,$$

so that from (3.22) we obtain

$$J dt = \hat{O}(p_2^{-4}) dt + \sum_b \hat{O}(p_2^{-4}) dB_t^b + d\hat{O}(p_2^{-3}) .$$

This together with (3.17) and (3.21) finally shows that

$$dp_2 = - \left(\frac{\alpha}{p_2^3} + \hat{O}(p_2^{-4}) \right) dt + \sum_b \left(\frac{\sqrt{2\gamma_b T_b} W_b}{p_2^2} + \hat{O}(p_2^{-3}) \right) dB_t^b + d \left(-\frac{\Phi_2}{p_2} + \hat{O}(p_2^{-2}) \right) ,$$

which implies (3.9) and completes the proof of Proposition 3.4.

Remark 3.10. We can argue (in a nonrigorous way) that when $|p_2|$ is very large, the dynamics of \tilde{p}_2 is approximately that of a particle interacting with two “effective” heat baths at temperatures T_1 and T_3 , but with some coupling of magnitude p_2^{-4} . Indeed, we can write (3.9) in the canonical “Langevin” form

$$d\tilde{p}_2(t) = \sum_b \left(-\tilde{\gamma}_b(X_t) \tilde{p}_2(t) dt + \sigma_b(X_t) dB_t^b \right) ,$$

with $\sigma_b(q, p) = \sqrt{2\gamma_b T_b} W_b / p_2^2 + \hat{O}(p_2^{-3})$ as in Proposition 3.4 and $\tilde{\gamma}_b(q, p) = \gamma_b \langle W_b^2 \rangle / p_2^4 + \hat{O}(p_2^{-5})$. We would like to introduce an effective temperature \tilde{T}_b by some Einstein-Smoluchowski relation of the kind $\sigma_b^2 / (2\tilde{\gamma}_b) = \tilde{T}_b$ in the limit $|p_2| \rightarrow \infty$. Unfortunately,

$$\lim_{|p_2| \rightarrow \infty} \frac{\sigma_b^2}{2\tilde{\gamma}_b} = \frac{W_b^2}{\langle W_b^2 \rangle} T_b ,$$

³For example if $W_b = -\cos(q_2 - q_b)$, there are in $\langle J \rangle$ some terms of the kind $\langle p_3 \cos(q_2 - q_1) \sin(q_2 - q_3) \rangle$ and $\langle p_1 \sin(q_2 - q_1) \cos(q_2 - q_3) \rangle$ which are non-zero.

which instead of a constant is an oscillatory quantity (with mean T_b). Now observe that these oscillations disappear if we approximate the oscillatory term W_b in σ_b by its quadratic mean $\langle W_b^2 \rangle^{1/2}$. This approximation is reasonable in the following sense: for small t and large $|p_2|$, we have that $p_2(s) \approx p_2(0)$ for $s \leq t$, so that

$$\int_0^t \frac{\sqrt{2\gamma_b T_b} W_b}{p_2^2(s)} dB_s^b \approx \frac{\sqrt{2\gamma_b T_b}}{p_2^2(0)} \langle W_b^2 \rangle^{1/2} M(t) \quad \text{with } M(t) = \int_0^t \frac{W_b}{\langle W_b^2 \rangle^{1/2}} dB_s^b.$$

But then, by the Dambis-Dubins-Schwarz representation theorem, there is another Brownian motion \tilde{B}^b such that $M(t) = \tilde{B}_{\tau(t)}^b$ with $\tau(t) = \int_0^t W_b^2 / \langle W_b^2 \rangle ds$. Clearly, when $|p_2|$ is very large, $\tau(t) \approx t$ so that $M(t)$ is very close to \tilde{B}_t^b . In this sense, when $|p_2| \rightarrow \infty$, it is reasonable to approximate $(\sqrt{2\gamma_b T_b} W_b / p_2^2) dB_s^b$ with $(\sqrt{2\gamma_b T_b} \langle W_b^2 \rangle^{1/2} / p_2^2) d\tilde{B}_s^b$, so that the Einstein-Smoluchowski relation indeed holds with effective temperature $\tilde{T}_b = T_b$.

Remark 3.11. The ergodicity of 1D Langevin processes is well understood: for any $\delta \in (-1, 0)$, processes satisfying an SDE of the kind

$$dp \sim -C_1 p^\delta dt + C_2 dB_t$$

asymptotically (when $|p| \rightarrow \infty$) are typically ergodic with a rate bounded above and below by $\exp(-c_\pm t^{(1+\delta)/(1-\delta)})$ for some constants $c_+, c_- > 0$ (see [3, 7] and references therein, in particular [7] for the lower bound). As argued in Remark 3.10, the variable \tilde{p}_2 (which is expected to be the component of the system that limits the convergence rate) essentially obeys an equation of the kind $dp \sim -C_1 p^{-3} dt + C_2 p^{-2} dB_t$ asymptotically. It is easy to check that a change of variable $y = p^3$ yields the asymptotic dynamics $dy \sim -C'_1 y^{-1/3} dt + C'_2 dB_t$ so that with $\delta = -1/3$, we expect a rate $\exp(-ct^{1/2})$. This suggests that the rate of convergence we find is optimal.

4 Lyapunov function

We now prove Proposition 2.2. Throughout this section, \tilde{p}_2 is the function defined in Proposition 3.4. The basic idea is to consider a Lyapunov function

$$V \sim \varrho(p) \tilde{p}_2^2 e^{\frac{\beta}{2} \tilde{p}_2^2} + e^{\beta H},$$

where $\varrho(p)$ is non-zero only when $|p_2|$ is much larger than $|p_1|$ and $|p_3|$. We will obtain that $LV \lesssim -\varphi(V)$, with $\varphi(s) \sim s/\log(s)$ as in Proposition 2.2. The fact that we do *not* have a bound of the kind $LV \lesssim -cV$ (which would yield exponential ergodicity) comes from the very slow decay of p_2 . The basic idea is that, when $p_2 \rightarrow \infty$ and $p_1, p_3 \sim 0$,

$$L\tilde{p}_2 \sim -p_2^{-3}, \quad \text{so that} \quad L\left(\tilde{p}_2^2 e^{\frac{\beta}{2} \tilde{p}_2^2}\right) \sim -e^{\frac{\beta}{2} \tilde{p}_2^2} \sim -\frac{V}{p_2^2} \sim -\frac{V}{\log V}.$$

We now introduce the necessary tools to make this observation rigorous.

Lemma 4.1. *For $\beta > 0$ small enough, there are constants $C_1, C_2 > 0$ such that*

$$Le^{\beta H} \leq (C_1 - C_2(p_1^2 + p_3^2))e^{\beta H}.$$

Proof. We have $Le^{\beta H} = \sum_b (-\gamma_b \beta (1 - \beta T_b) p_b^2 + \beta \tau_b p_b + \gamma_b \beta T_b) e^{\beta H}$. If $\beta < 1/\max(T_1, T_3)$, then $\gamma_b \beta (1 - \beta T_b) > 0$. Moreover, since $\beta \tau_b p_b < \frac{1}{2} \gamma_b \beta (1 - \beta T_b) p_b^2 + C$ for C large enough, we find the desired bound. \square

Lemma 4.2. For $\beta > 0$ small enough, there is a constant $C_3 > 0$ such that on $\Omega^\dagger = \{x \in \Omega : p_2 \neq 0\}$,

$$L(\tilde{p}_2^2 e^{\frac{\beta}{2}\tilde{p}_2^2}) \leq (-C_3 + \hat{O}(p_2^{-1}))e^{\frac{\beta}{2}\tilde{p}_2^2}. \quad (4.1)$$

Proof. Introducing $f(s) = s^2 e^{\frac{\beta}{2}s^2}$, we have by the Itô formula and Proposition 3.4 that

$$\begin{aligned} d(\tilde{p}_2^2 e^{\frac{\beta}{2}\tilde{p}_2^2}) &= df(\tilde{p}_2) = f'(\tilde{p}_2)(a dt + \sum_b \sigma_b dB_t^b) + \frac{1}{2}f''(\tilde{p}_2) \sum_b \sigma_b^2 dt \\ &= (2\tilde{p}_2 + \beta\tilde{p}_2^3)e^{\frac{\beta}{2}\tilde{p}_2^2}(a dt + \sum_b \sigma_b dB_t^b) + \frac{1}{2}(2 + 5\beta\tilde{p}_2^2 + \beta^2\tilde{p}_2^4)e^{\frac{\beta}{2}\tilde{p}_2^2} \sum_b \sigma_b^2 dt. \end{aligned}$$

Now since $a = -\alpha p_2^{-3} + \hat{O}(p_2^{-4})$ with $\alpha = \sum_b \gamma_b \langle W_b^2 \rangle$, $\sigma_b = \sqrt{2\gamma_b T_b} W_b p_2^{-2} + \hat{O}(p_2^{-3})$, and $\tilde{p}_2^k = p_2^k + \hat{O}(p_2^{k-1})$ for all k , we find after taking the expectation value

$$L(\tilde{p}_2^2 e^{\frac{\beta}{2}\tilde{p}_2^2}) = (-\alpha\beta + \beta^2 \sum_b \gamma_b T_b W_b^2 + \hat{O}(p_2^{-1}))e^{\frac{\beta}{2}\tilde{p}_2^2},$$

which gives the desired bound if β is small enough (recall that the W_b^2 are bounded). \square

Convention: We fix $\beta > 0$ small enough so that the conclusions of Lemma 4.1 and Lemma 4.2 hold.

Let $k \geq 1$ be an integer and $R > 0$ be a constant (which we will fix later). We split Ω into three disjoint sets $\Omega_1, \Omega_2, \Omega_3$ defined by

- $\Omega_1 = \{x \in \Omega : |p_2| < (p_1^2 + p_3^2)^k + R\}$,
- $\Omega_2 = \{x \in \Omega : (p_1^2 + p_3^2)^k + R \leq |p_2| \leq 2(p_1^2 + p_3^2)^k + 2R\}$,
- $\Omega_3 = \{x \in \Omega : |p_2| > 2(p_1^2 + p_3^2)^k + 2R\}$.

Fix some $m, n \in \mathbb{N}$ and $\ell \geq 1$. On $\Omega_2 \cup \Omega_3$, we have by definition $|p_2| \geq (p_1^2 + p_3^2)^k + R$, so that

$$\left| \frac{p_1^n p_3^m}{p_2^\ell} \right| \leq \frac{|p_1^n p_3^m|}{((p_1^2 + p_3^2)^k + R)^\ell} \quad (\text{on } \Omega_2 \cup \Omega_3).$$

Clearly, if k and R are large enough, the right-hand side is bounded by an arbitrarily small constant. Therefore, any given $\hat{O}(p_2^{-1})$ is also bounded by an arbitrarily small constant on $\Omega_2 \cup \Omega_3$ provided that k and R are large enough, since it is by definition a sum *finitely* many terms of order less or equal to -1. Using this, we obtain

Lemma 4.3. For k and R large enough, there are constants $C_4, \dots, C_7 > 0$ such that the following properties hold on $\Omega_2 \cup \Omega_3$:

$$|\tilde{p}_2^2 - p_2^2| < C_4, \quad (4.2)$$

$$L(\tilde{p}_2^2 e^{\frac{\beta}{2}\tilde{p}_2^2}) \leq -C_5 e^{\frac{\beta}{2}\tilde{p}_2^2}, \quad (4.3)$$

$$C_6 e^{-\frac{\beta}{2}(p_1^2 + p_3^2)} e^{\beta H} \leq e^{\frac{\beta}{2}\tilde{p}_2^2} \leq C_7 e^{-\frac{\beta}{2}(p_1^2 + p_3^2)} e^{\beta H}. \quad (4.4)$$

Proof. Since $\tilde{p}_2 = p_2 + \Phi_2(q)/p_2 + \hat{O}(p_2^{-2})$, we have $\tilde{p}_2^2 = p_2^2 + 2\Phi_2(q) + \hat{O}(p_2^{-1})$. By taking k large enough, the $\hat{O}(p_2^{-1})$ here is bounded by a constant on the set $\Omega_2 \cup \Omega_3$, which implies (4.2). Moreover, for large k and R , the $\hat{O}(p_2^{-1})$ in (4.1) is also bounded on $\Omega_2 \cup \Omega_3$ by an arbitrarily small constant, which implies (4.3). To prove (4.4), observe that

$$e^{\frac{\beta}{2}\tilde{p}_2^2} = e^{\frac{\beta}{2}(\tilde{p}_2^2 - p_2^2 - p_1^2 - p_3^2 - U(q))} e^{\beta H},$$

where $U(q)$ contains all the potentials appearing in H . This together with the boundedness of U and (4.2), implies (4.4). \square

Convention: We fix k and R such that the conclusions of Lemma 4.3 hold.

Definition 4.4. Let $\chi : \mathbb{R} \rightarrow [0, 1]$ be a smooth function such that $\chi(s) = 0$ when $|s| < 1$ and $\chi(s) = 1$ when $|s| > 2$. We introduce the cutoff function

$$\varrho(p) = \chi\left(\frac{p_2}{(p_1^2 + p_3^2)^k + R}\right),$$

and the Lyapunov function

$$V = 1 + A\varrho(p)\tilde{p}_2^2 e^{\frac{\beta}{2}\tilde{p}_2^2} + e^{\beta H},$$

with $A > 0$ (to be chosen later).

By construction $\varrho(p)$ is smooth, $\varrho(p) = 0$ on Ω_1 and $\varrho(p) = 1$ on Ω_3 , with some transition on Ω_2 . Remember that \tilde{p}_2 is by construction smooth on Ω^\dagger , i.e., when $p_2 \neq 0$. In particular, since $\Omega_2 \cup \Omega_3 \subset \Omega^\dagger$, the function $\varrho(p)\tilde{p}_2^2 e^{\frac{\beta}{2}\tilde{p}_2^2}$ is smooth on Ω , and so is V . We can now finally give the

Proof of Proposition 2.2. We show here that V satisfies the conditions enumerated in Proposition 2.2 if A is large enough. Let us first prove the first statement, which is that there exist $c_1, c_2 > 0$ such that

$$1 + c_1 e^{\beta H} \leq V \leq c_2(1 + p_2^2) e^{\beta H}. \quad (4.5)$$

Clearly the lower bound on V holds. We now prove the upper bound. Throughout the proof, we denote by c a generic positive constant which can be each time different. Since $\varrho \neq 0$ only on $\Omega_2 \cup \Omega_3$, we have by (4.2) and (4.4),

$$\begin{aligned} |A\varrho(p)\tilde{p}_2^2 e^{\frac{\beta}{2}\tilde{p}_2^2}| &\leq c(p_2 + C_4)^2 e^{-\frac{\beta}{2}(p_1^2 + p_3^2)} e^{\beta H} \\ &\leq c(p_2^2 + 2C_4 p_2 + C_4^2) e^{\beta H} \leq c(1 + p_2^2) e^{\beta H}. \end{aligned}$$

But then $V \leq 1 + c(1 + p_2^2) e^{\beta H} \leq c(1 + p_2^2) e^{\beta H}$, where the last inequality holds because H is bounded below, so that $e^{\beta H}$ is bounded away from zero.

Let us now move to the second statement of Proposition 2.2, which is that for c_3, c_4 large enough and a compact set K ,

$$LV \leq c_3 \mathbf{1}_K - \varphi(V) \quad \text{with } \varphi(s) = \frac{c_4 s}{2 + \log(s)}. \quad (4.6)$$

We first show that

$$LV \leq c \mathbf{1}_K - c e^{\beta H} \quad \text{with } K = \{x \in \Omega_1 \cup \Omega_2 : p_1^2 + p_3^2 \leq M\}, \quad (4.7)$$

for some large enough M . Clearly K is compact, since $\Omega_1 \cup \Omega_2 = \{x \in \Omega : |p_2| \leq 2(p_1^2 + p_3^2)^k + 2R\}$.

- On Ω_1 we simply have $V = 1 + e^{\beta H}$. By Lemma 4.1, we have $LV \leq (C_1 - C_2(p_1^2 + p_3^2))e^{\beta H}$. Since $\Omega_1 \setminus K = \{x \in \Omega_1 : p_1^2 + p_3^2 > M\}$, we have for large enough M that $LV \leq -c e^{\beta H}$ on $\Omega_1 \setminus K$, and therefore (4.7) holds on Ω_1 .
- On Ω_2 , the key is to observe that there is a polynomial $z(p_1, p_2, p_3)$ such that

$$|L(A\varrho(p)\tilde{p}_2^2 e^{\frac{\beta}{2}\tilde{p}_2^2})| \leq z(p) e^{\frac{\beta}{2}\tilde{p}_2^2} \leq C_7 z(p) e^{-\frac{\beta}{2}(p_1^2 + p_3^2)} e^{\beta H},$$

where the second inequality comes from (4.4). Now, since $p_1^2 + p_2^2 \sim |p_2|^{1/k}$ on Ω_2 , we have that $z(p) e^{-\frac{\beta}{2}(p_1^2 + p_3^2)}$ is bounded on Ω_2 . Therefore, by this and Lemma 4.1, we have on Ω_2 ,

$$\begin{aligned} LV &\leq \left(C_7 z(p) e^{\frac{\beta}{2}(-p_1^2 - p_3^2)} + C_1 - C_2(p_1^2 + p_3^2)\right) e^{\beta H} \\ &\leq (c - C_2(p_1^2 + p_3^2)) e^{\beta H}. \end{aligned}$$

which, as in the previous case, implies that (4.7) holds on Ω_2 if M is large enough.

- On Ω_3 , which is the critical region, we have $V = 1 + A\tilde{p}_2^2 e^{\frac{\beta}{2}\tilde{p}_2^2} + e^{\beta H}$. By Lemma 4.1 and (4.3), it holds in Ω_3 that

$$LV \leq (C_1 - C_2(p_1^2 + p_3^2))e^{\beta H} - C_5 A e^{\frac{\beta}{2}\tilde{p}_2^2}. \quad (4.8)$$

On the set $\{x \in \Omega_3 : C_1 - C_2(p_1^2 + p_3^2) \leq -1\}$, we simply have $LV \leq -e^{\beta H}$, so that (4.7) holds trivially. On the other hand, on the set $\{x \in \Omega_3 : C_1 - C_2(p_1^2 + p_3^2) > -1\}$ the quantity $p_1^2 + p_3^2$ is bounded, so that $e^{\frac{\beta}{2}\tilde{p}_2^2} \geq ce^{\beta H}$ by (4.4), which with (4.8) implies that

$$LV \leq (C_1 - C_2(p_1^2 + p_3^2))e^{\beta H} - cAe^{\beta H} \leq (C_1 - cA)e^{\beta H}.$$

By making A large enough, we again find a bound $LV \leq -ce^{\beta H}$, so that (4.7) holds.

Therefore, (4.7) holds on all of Ω . To obtain (4.6), we need only show that $e^{\beta H} \geq cV/(2 + \log V)$. By the boundedness of the potentials and the definition of V , we have $1 + p_2^2 \leq 2H + c \leq c \log(e^{\beta H}) + c \leq c \log V + c \leq c(\log V + 2)$. But then by (4.5) we indeed have that $e^{\beta H} \geq cV/(1 + p_2^2) \geq cV/(2 + \log V)$. This completes the proof of Proposition 2.2. \square

Remark 4.5. The external forces τ_b and the pinning potentials U_i (if non-zero) do not play a central role in the properties of the Lyapunov function. On the contrary, the interaction potentials W_b are very important, since we need $\alpha = \sum_b \gamma_b \langle W_b^2 \rangle$ to be strictly positive.

Remark 4.6. Although we assume throughout that T_1 and T_3 are strictly positive, the computations that lead to the Lyapunov function apply to zero temperatures as well (the temperatures only appear in some non-dominant terms in V and LV). In that case, the existence of an invariant measure can still be obtained by compactness arguments (see e.g., Proposition 5.1 of [8]). However, the smoothness, uniqueness and convergence assertions do not necessarily hold: when $T_1 = T_3 = 0$ the system is deterministic, the transition probabilities are not smooth, and there is at least one invariant measure concentrated at each stationary point of the system. The positive temperatures assumption is crucial in the next section.

5 Smoothness and irreducibility

This section is devoted to proving that the hypotheses of Theorem 2.1 other than the existence of the Lyapunov function are satisfied. More precisely we will prove the following proposition.

Proposition 5.1. *The following properties hold.*

- (i) *The transition probabilities $P^t(x, \cdot)$ have a density $p_t(x, y)$ that is smooth in (t, x, y) when $t > 0$. In particular, the process is strong Feller.*
- (ii) *The time-1 skeleton $(X_n)_{n=0,1,2,\dots}$ is irreducible, and the Lebesgue measure m on (Ω, \mathcal{B}) is a maximal irreducibility measure.*
- (iii) *Every compact set is petite.*

In a sense, (i) shows that we have some effective diffusion in all directions at very short times, and (ii) shows that every part of the phase space is eventually reached with positive probability. Observe that (iii) follows from (i) and (ii). Indeed, by (i), (ii) and Proposition 6.2.8 of [11], every compact set is petite for the time-1 skeleton. But then every compact set is also petite with respect to the process X_t (simply by choosing a sampling measure on $[0, \infty)$ that is concentrated on \mathbb{N}). Therefore, we need only prove (i) and (ii), which we do in the next two subsections.

5.1 Smoothness

We show here that the semigroup has a smoothing effect. More specifically, we show that a Hörmander bracket condition is satisfied, so that the transition probability $P^t(x, dy)$ has a density $p_t(x, y)$ that is smooth in t, x and y , and every invariant measure has a smooth density [9].

We identify vector fields over Ω and the corresponding first-order differential operators in the usual way (we identify the tangent space of Ω with \mathbb{R}^6). This enables us to consider Lie algebras of vector fields over Ω of the kind $\sum_i (f_i(q, p)\partial_{q_i} + g_i(q, p)\partial_{p_i})$, where the Lie bracket $[\cdot, \cdot]$ is the usual commutator of two operators.

Definition 5.2. We define \mathcal{M} as the smallest Lie algebra that

- (i) contains the constant vector fields $\partial_{p_1}, \partial_{p_3}$,
- (ii) is closed under the operation $[\cdot, A_0]$, where

$$A_0 = \sum_{i=1}^3 (p_i \partial_{q_i} - u_i \partial_{p_i}) + \sum_b (w_b (\partial_{p_b} - \partial_{p_2}) + \tau_b \partial_{p_b} - \gamma_b p_b \partial_{p_b})$$

is the drift part of L .

By the definition of a Lie algebra, \mathcal{M} is closed under linear combinations and Lie brackets.

Lemma 5.3. Hörmander's bracket condition is satisfied. More precisely, for all $x = (q, p)$, the set $\{v(x) : v \in \mathcal{M}\}$ spans \mathbb{R}^6 .

Proof. By definition, the constant vector fields ∂_{p_1} and ∂_{p_3} belong to \mathcal{M} . Moreover, for $b = 1, 3$, $[\partial_{p_b}, A_0] = \partial_{q_b} - \gamma_b \partial_{p_b}$. Since \mathcal{M} is closed under linear combinations and $\partial_{p_b} \in \mathcal{M}$, it follows that $\partial_{q_b} \in \mathcal{M}$ for $b = 1, 3$. Thus it only remains to show that at each $x \in \Omega$, we can span the directions of ∂_{q_2} and ∂_{p_2} . In the following, f denotes a generic function on Ω that can be each time different. We have $[\partial_{q_b}, A_0] = w'_b(q_2 - q_b)\partial_{p_2} + f(q)\partial_{p_b}$ so that commuting $n - 1$ times with ∂_{q_b} we get that for all $n \geq 1$

$$w_b^{(n)}(q_2 - q_b)\partial_{p_2} + f(q)\partial_{p_b} \in \mathcal{M}. \quad (5.1)$$

Commuting the above with A_0 , we find that for all $n \geq 1$,

$$w_b^{(n)}(q_2 - q_b)\partial_{q_2} + f(q, p)\partial_{p_2} + f(q)\partial_{p_b} + f(q, p)\partial_{q_b} \in \mathcal{M}. \quad (5.2)$$

By Assumption 1.2, there is some $b \in \{1, 3\}$ such that for any fixed $x \in \Omega$, there is an integer $n \geq 1$ such that $w_b^{(n)}(q_2 - q_b) \neq 0$. Thus, by (5.1) and (5.2) the proof is complete. \square

Thus, we have proved Proposition 5.1 (i).

5.2 Irreducibility

We show in this section that the process has an irreducible skeleton. We give in fact two different proofs. The first one is given in a general and abstract framework, and works for chains of any lengths. The second one is more explicit, gives more than the irreducibility of a skeleton, but relies strongly on the fact that the chain is made of only three rotors.

5.2.1 Abstract version

Consider the transition probabilities $\tilde{P}^t(\cdot, \cdot)$ of the system at equilibrium, *i.e.*, with parameters $\tau_1 = \tau_3 = 0$ and $T_1 = T_3 = T$ for some $T > 0$. For all x and t , the measures $P^t(x, \cdot)$ and $\tilde{P}^t(x, \cdot)$ are equivalent. This equivalence holds because any change of the parameters τ_1, τ_3 (respectively T_1, T_3) can be absorbed by shifting (respectively scaling) the Brownian motions appropriately. Therefore, it is enough to prove the irreducibility claim at equilibrium.

At equilibrium, the Gibbs measure ν with density $\frac{1}{Z} \exp(-H/T)$ is invariant (with some normalisation constant Z) as mentioned earlier. Note that we do not assume *a priori* that ν is the unique invariant measure at equilibrium, nor that the system at equilibrium is irreducible. The only two properties that we need are invariance and (everywhere) positiveness of the density of ν .

Lemma 5.4. *The equilibrium transition probabilities satisfy the following property: for every measurable set S one has for all t*

$$\int_S \tilde{P}^t(x, S^c) d\nu = \int_{S^c} \tilde{P}^t(x, S) d\nu.$$

Proof. We have by the invariance of ν ,

$$\begin{aligned} \int_{S^c} \tilde{P}^t(x, S) d\nu - \int_S \tilde{P}^t(x, S^c) d\nu &= \int_{S^c} \tilde{P}^t(x, S) d\nu + \int_S (\tilde{P}^t(x, S) - 1) d\nu \\ &= \int_{\Omega} \tilde{P}^t(x, S) d\nu - \int_S 1 d\nu = \nu(S) - \nu(S) = 0, \end{aligned}$$

which completes the proof. \square

Lemma 5.5. *Let A be a closed set. If A is invariant under \tilde{P}^1 (*i.e.*, $\tilde{P}^1(x, A) = 1$ for all $x \in A$), then either $A = \emptyset$ or $A = \Omega$.*

Proof. By Lemma 5.4, $\int_{A^c} \tilde{P}^1(x, A) d\nu = \int_A \tilde{P}^1(x, A^c) d\nu = 0$ since $\tilde{P}^1(x, A^c) = 0$ for all $x \in A$. This implies that $\tilde{P}^1(x, A) = 0$ for all $x \in A^c$, since $x \mapsto \tilde{P}^1(x, A)$ is continuous on the open set A^c and ν has an everywhere positive density. But then $\tilde{P}^1(x, A)$ is 1 when $x \in A$ and 0 when $x \in A^c$, so that by continuity we have $\partial A = \emptyset$. Since Ω is connected, the conclusion follows. \square

Note that same does not hold for non-closed sets: for example Ω minus any set of zero Lebesgue measure is still an invariant set.

Lemma 5.6. *The time-1 skeleton $(X_n)_{n=0,1,2,\dots}$ is irreducible, and the Lebesgue measure m is a maximal irreducibility measure.*

Proof. As discussed above, it is enough to prove the result at equilibrium, *i.e.*, with $\tilde{P}^1(\cdot, \cdot)$. Let B be a set such that $m(B) > 0$. We need to show that the set $A = \{x \in \Omega : \sum_{n=1}^{\infty} \tilde{P}^n(x, B) = 0\}$ is empty. By the smoothness of $x \mapsto \tilde{P}^n(x, B)$, it is easy to see that $A^c = \{x \in \Omega : \exists n > 0, \tilde{P}^n(x, B) > 0\}$ is open, so that A is closed. Moreover, for all $x \in A$ it holds that $0 = \sum_{n=1}^{\infty} \tilde{P}^n(x, B) \geq \sum_{n=1}^{\infty} \tilde{P}^{n+1}(x, B) = \int_{\Omega} \tilde{P}^1(x, dy) \sum_{n=1}^{\infty} \tilde{P}^n(y, B)$. But since by the definition of A we have $\sum_{n=1}^{\infty} \tilde{P}^n(y, B) > 0$ for all $y \in A^c$, we must have $\tilde{P}^1(x, A^c) = 0$ for all $x \in A$, so that A is invariant. But then by Lemma 5.5 either $A = \emptyset$ or $A = \Omega$. We need to eliminate the second possibility. Since $m(B) > 0$ and ν has positive density, we have $\nu(B) > 0$. By the invariance of ν , we have $\int_{\Omega} \tilde{P}^1(x, B) d\nu = \nu(B) > 0$. But then there is some $x \in \Omega$ such that $\tilde{P}^1(x, B) > 0$, so that $x \in A^c$. Therefore $A \neq \Omega$, and thus $A = \emptyset$ and the process is irreducible with measure m . That m is a maximal irreducibility measure follows immediately from the fact that the transition probabilities are absolutely continuous with respect to m . This completes the proof. \square

Thus, we have proved Proposition 5.1(ii), so that the proof of Proposition 5.1 is complete.

5.2.2 Direct control version

We give now an alternate proof of Proposition 5.1(ii). We establish the irreducibility of our process by using controllability arguments. We aim to establish the controllability of (1.1), where the Brownian motions B_t^1 and B_t^3 are replaced with some deterministic, smooth controls $f_b : \mathbb{R}^+ \rightarrow \mathbb{R}$. By absorbing some terms into the controls f_b , this problem is obviously equivalent to controlling the differential equation

$$\begin{aligned}\dot{q}_i(t) &= p_i(t) , \\ \dot{p}_2(t) &= - \sum_b w_b(q_2(t) - q_b(t)) , \\ \dot{p}_b(t) &= f_b(t) .\end{aligned}\tag{5.3}$$

In [5] the irreducibility of chains oscillators has been studied. The authors have proved that chains of any length are controllable in arbitrarily small times. This is of course not the case in our model: since the force applied to p_2 is bounded by some constants

$$K^- = \sum_b \min_{s \in \mathbb{T}} w_b(s), \quad K^+ = \sum_b \max_{s \in \mathbb{T}} w_b(s) ,$$

the minimal time we need to bring the system from $x^i = (q^i, p^i)$ to $x^f = (q^f, p^f)$ is at best proportional to $|p_2^f - p_2^i|$. On the other hand, q_1, p_1, q_3, p_3 can be put into any position in arbitrarily short time. Observe that due to Assumption 1.2 and the fact that $\langle w_b \rangle = 0$, we have $K^- < 0 < K^+$. We will prove the following proposition (remember that the positions q_i are defined modulo 2π).

Proposition 5.7. *The system (5.3) is approximately controllable in the sense that for all $x^i = (q^i, p^i)$, $x^f = (q^f, p^f)$ and all $\varepsilon > 0$, there is a time $T^* > 0$ satisfying $T^* \leq c_1 + c_2|p_2^f - p_2^i|$ for some constants c_1 and c_2 such that for all $T > T^*$ there are some smooth controls $f_1, f_3 : [0, T] \rightarrow \mathbb{R}$ such that the solution of (5.3) with initial condition x^i satisfies $\|x(T) - x^f\| < \varepsilon$.*

This property implies the irreducibility of the chain, since the classical result of Stroock and Varadhan [15] links the support of the semigroup P^t and the accessible points for (5.3), and implies in particular that for all $x^i = (q^i, p^i)$ and $t > c_1$ the subspace $\{x \in \Omega : |p_2 - p_2^i| \leq (t - c_1)/c_2\}$ is included in the support of $P^t(x^i, \cdot)$.

The idea is the following: in the next lemma, we show how the middle rotor can be forced into any configuration by applying some piecewise constant force $g(t)$ to it, with $g(t) \in [K^-, K^+]$. Then, we will argue that one can move q_1 and q_3 (on which we have good control) in such a way that the force exerted on the middle rotor is almost $g(t)$.

Lemma 5.8. *Consider the system*

$$\begin{aligned}\dot{\bar{q}}_2(t) &= \bar{p}_2(t) , \\ \dot{\bar{p}}_2(t) &= g(t) - u_2(\bar{q}_2(t)) ,\end{aligned}\tag{5.4}$$

and fix some initial and terminal conditions (q_2^i, p_2^i) and (q_2^f, p_2^f) . We claim that there is a T^ satisfying $T^* \leq c_1 + c_2|p_2^f - p_2^i|$ for some constants c_1 and c_2 such that for all $T > T^*$ there is a piecewise constant control $g(t) : \mathbb{R}^+ \rightarrow [K^-, K^+]$ (with finitely many constant pieces) such that the solution of (5.4) with initial data (q_2^i, p_2^i) satisfies $\bar{p}_2(T) = p_2^f$ and $\bar{q}_2(T) = q_2^f$.*

Proof. We prove this result only in the case $u_2 \equiv 0$. If $p_2^f \geq p_2^i$, then let $\Theta = (p_2^f - p_2^i)/K^+$ and let $g(t) = K^+$ for all $t \in [0, \Theta]$. If $p_2^f < p_2^i$ let $\Theta = (p_2^f - p_2^i)/K^-$ and let $g(t) = K^-$ for all $t \in [0, \Theta]$. In both cases, $\bar{p}_2(\Theta) = p_2^f$, while $\bar{q}_2(\Theta)$ might be anything. Let now $K^* = \min(|K^+|, |K^-|)$, and

consider some $\Delta > 0$ and $a \in [0, K^*]$. Assume that $g(t) = a$ when $t \in [\Theta, \Theta + \Delta)$ and $g(t) = -a$ when $t \in [\Theta + \Delta, \Theta + 2\Delta]$. Clearly $\bar{p}_2(\Theta + 2\Delta) = \bar{p}_2(\Theta) = p_2^f$ and

$$\bar{q}_2(\Theta + 2\Delta) = \bar{q}_2(\Theta) + 2\Delta p_2^f + a\Delta^2.$$

Observe that as soon as $\Delta > \sqrt{2\pi/K^*}$, we can choose $a \in [0, K^*]$ so that $\bar{q}_2(\Theta + 2\Delta)$ takes any value (modulo 2π). In particular, we can choose it to be q_2^f , so that we have the advertised result with $T^* = \Theta + \sqrt{2\pi/K^*}$. \square

Remark 5.9. We have given a proof only if $u_2 \equiv 0$. However, the result remains true even if $u_2 \neq 0$, although the proof is much more involved. Typically, if the pinning is stronger than the interaction forces w_b , and the initial condition is such that p_2 is small, we sometimes have to push the middle rotor several times back and forth to increase its energy enough to pass above the “potential barrier” created by U_2 . Conversely, we sometimes have to brake the middle rotor with some non-trivial controls.

We now have some piecewise constant control $g(t)$ that can bring the middle rotor to the final configuration of our choice. It remains to show that we can make the external rotors follow some trajectories that have the appropriate initial and terminal conditions, and such that the force exerted on the middle rotator closely approximates $g(t)$. We do not prove this in detail, but we list here the main steps.

- Since $K^- \leq g(t) \leq K^+$, it is possible to find piecewise smooth functions $q_b^*(t)$, $b = 1, 3$, such that $\sum_b w_b(\bar{q}_2(t) - q_b^*(t)) \equiv g(t)$, where $\bar{q}_2(t)$ is the solution of (5.4).
- Let $\delta > 0$ be small. We can find some smooth trajectories $q_b(t)$ compatible with the boundary conditions x^i and x^f , such that $q_b(t) = q_b^*(t)$ for all $t \in [0, T] \setminus A_\delta$, where A_δ consists of a finite number of intervals of total length at most δ . We can choose the controls f_b so that the $q_b(t)$ constructed here are solutions to (5.3) (when δ is small, $f_b(t)$ is typically very large for $t \in A_\delta$).
- Since the interaction forces w_b are bounded, their effect during the times $t \in A_\delta$ is negligible when δ is small. More precisely, it can be shown that the solution $q_2(t)$ and $p_2(t)$ of (5.3) converge uniformly on $[0, T]$ to the solutions $\bar{q}_2(t)$ and $\bar{p}_2(t)$ of (5.4) when $\delta \rightarrow 0$. Therefore, the system is approximately controllable in the sense of Proposition 5.7.

6 Numerical illustrations

In this section we illustrate some properties of the invariant measure in the case where $U_i \equiv 0$ and $W_1 = W_3 = -\cos$.

We use throughout the values $\gamma_1 = \gamma_3 = 1$ and $\tau_1 = 0$. We give examples of how the marginal distributions of p_1, p_2, p_3 depend on the temperatures T_1, T_3 and the external force τ_3 . We apply the numerical algorithm given in [10] with time-increment $h = 0.001$. The resulting graphs are quite independent of h . In order to obtain good statistics and smooth curves, the probability densities shown below are sampled over 10^8 units of time and several hundred bins.

At equilibrium, *i.e.*, when $T_1 = T_3 = T$ and $\tau_3 = 0$ (remember that $\tau_1 = 0$ in this section), the marginal law of each p_i has a density proportional to $\exp(-p_i^2/2T)$ for $i = 1, 2, 3$. This is obviously not the case out of equilibrium. Moreover, since we work with a finite number of rotors, we do not expect to see any form of local thermal equilibrium in the bulk of the chain (here the “bulk” consists of only the middle rotor). Clearly, the distribution of p_2 can be quite far from Maxwellian (Gaussian).

In Figure 2 we show the marginal distributions of p_1, p_2, p_3 for different temperatures and no external force. For each pair of temperatures, we show the distributions both in linear and logarithmic

scale. At equilibrium, when $T_1 = T_3 = 10$, all three distributions coincide exactly and are Gaussian. However, when $T_1 \neq T_3$, we see that the distribution of p_2 is not Gaussian (clearly, the distribution is not a parabola in logarithmic scale).

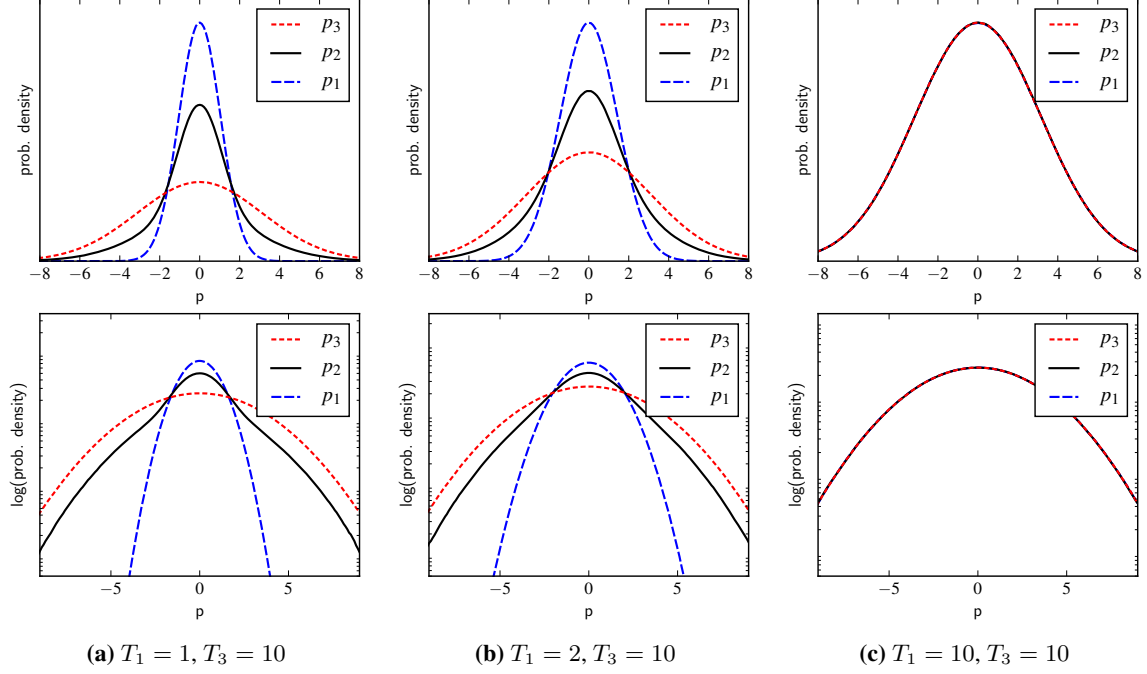


Figure 2 – Distribution of p_1, p_2, p_3 , with no external force and several temperatures.

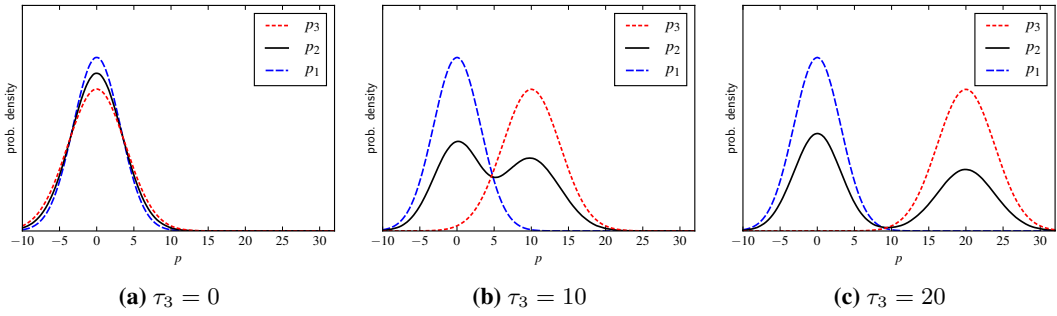


Figure 3 – Distribution of p_1, p_2, p_3 , with $T_1 = 10, T_3 = 15$ for 3 values of τ_3 .

We next consider the effect of the external force τ_3 on the marginal distributions of the p_i , for $T_1 = 10$ and $T_3 = 15$. As illustrated in Figure 3, the distributions of p_1 and p_3 are close to Gaussians with variance T_1 and T_3 and mean 0 and τ_3 . Note that when $\tau_3 \neq 0$, the distribution of p_2 has two maxima: one at 0 and one at τ_3 . The explanation for these two maxima can be found by looking at the trajectories $p_i(t)$ as shown in Figure 4 (for $\tau_3 = 20$); p_1 fluctuates around 0, p_3 fluctuates around τ_3 , and p_2 switches between these two regimes. In the regime where p_2 fluctuates around zero, the rotor 2 interacts strongly with 1 and weakly with 3 (since then the force w_3 oscillates with “high frequency” $p_3 - p_2 \sim \tau_3$). Inversely, in the regime where p_2 fluctuates around τ_3 , it interacts strongly with 3 and only weakly with 1. Other simulations (not shown here) show that, as expected, the larger τ_3 , the less frequent the switches between these two regimes. The asymmetry of the two maxima in Figure 3 is explained by the inequality $T_1 < T_3$, which makes the fluctuations larger in the second regime, so that the mean sojourn time there is shorter.

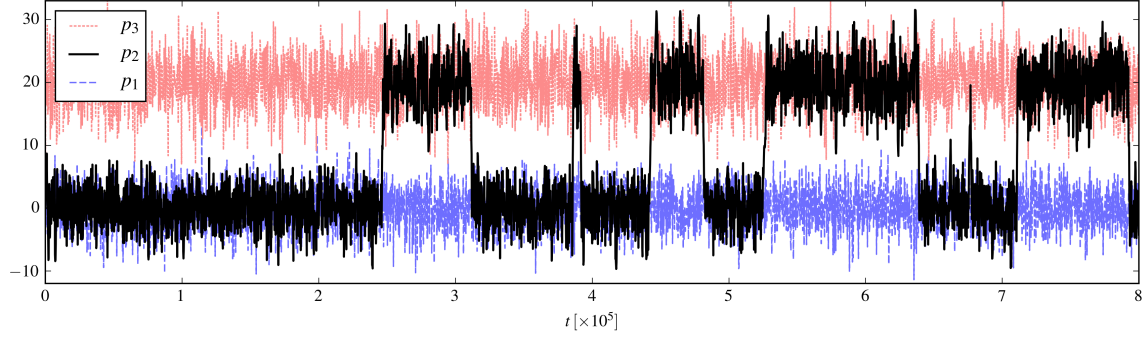


Figure 4 – Representation of the evolution of p_1, p_2, p_3 with $T_1 = 10, T_3 = 15, \tau_3 = 20$.

Note added in proof

Based on the results of this paper, an extension to four rotors has been obtained more recently [2].

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References

- [1] P. Carmona. Existence and uniqueness of an invariant measure for a chain of oscillators in contact with two heat baths. *Stochastic Process. Appl.* **117** (2007), 1076–1092.
- [2] N. Cuneo and J.-P. Eckmann. Non-equilibrium steady states for chains of four rotors (2015), arXiv preprint: 1504.04964.
- [3] R. Douc, G. Fort, and A. Guillin. Subgeometric rates of convergence of f -ergodic strong Markov processes. *Stochastic Process. Appl.* **119** (2009), 897–923.
- [4] J.-P. Eckmann and M. Hairer. Non-equilibrium statistical mechanics of strongly anharmonic chains of oscillators. *Comm. Math. Phys.* **212** (2000), 105–164.
- [5] J.-P. Eckmann, C.-A. Pillet, and L. Rey-Bellet. Entropy production in nonlinear, thermally driven Hamiltonian systems. *J. Statist. Phys.* **95** (1999), 305–331.
- [6] J.-P. Eckmann, C.-A. Pillet, and L. Rey-Bellet. Non-equilibrium statistical mechanics of anharmonic chains coupled to two heat baths at different temperatures. *Comm. Math. Phys.* **201** (1999), 657–697.
- [7] M. Hairer. How hot can a heat bath get? *Comm. Math. Phys.* **292** (2009), 131–177.
- [8] M. Hairer and J. C. Mattingly. Slow energy dissipation in anharmonic oscillator chains. *Comm. Pure Appl. Math.* **62** (2009), 999–1032.
- [9] L. Hörmander. Hypoelliptic second order differential equations. *Acta Math.* **119** (1967), 147–171.

- [10] A. Iacobucci, F. Legoll, S. Olla, and G. Stoltz. Negative thermal conductivity of chains of rotors with mechanical forcing. *Phys. Rev. E* **84** (2011), 061108.
- [11] S. Meyn and R. L. Tweedie. *Markov chains and stochastic stability* (Cambridge University Press, Cambridge, 2009), second edition. With a prologue by Peter W. Glynn.
- [12] S. P. Meyn and R. L. Tweedie. Stability of Markovian processes. III. Foster-Lyapunov criteria for continuous-time processes. *Adv. in Appl. Probab.* **25** (1993), 518–548.
- [13] L. Rey-Bellet and L. E. Thomas. Exponential convergence to non-equilibrium stationary states in classical statistical mechanics. *Comm. Math. Phys.* **225** (2002), 305–329.
- [14] J. A. Sanders, F. Verhulst, and J. Murdock. *Averaging methods in nonlinear dynamical systems*, volume 59 of *Applied Mathematical Sciences* (Springer, New York, 2007), second edition.
- [15] D. W. Stroock and S. R. S. Varadhan. On the support of diffusion processes with applications to the strong maximum principle. In: *Proceedings of the Sixth Berkeley Symposium on Mathematical Statistics and Probability, Vol. III: Probability theory* (Univ. California Press, Berkeley, Calif., 1972).
- [16] P. A. Vela. Averaging and control of nonlinear systems. Ph.D. thesis, California Institute of Technology (2003).